PLS-2 Example

This example shows how to compute Partial Least Squares (PLS) predictions with multiple constituents. Computing PLS for multiple constituents is known as PLS-2.

PLS can be computed with and without pre-processing. For PLS, pre-processing consists of mean-centering, which means to subtract out the mean from the data. This example shows how to compute PLS-2 with and without mean-centering.

PLS Algorithm

The PLS Algorithm is encapsulated in the following MATLAB function. If `meanCentered` is not entered, or if it is false, then pre-processing (mean centering) is not done. If `meanCentered` is true, then pre-processiing (mean centering) is done.

```
function [C_pls, B_pls] = pnnl_pls(A_train, C_train, A_unknown, nLatentVariables, meanCentered)
    %pnnl_pls Partial least squares (PLS) regression
    %
    %   [C_pls, B_pls] = pnnl_pls(A_train, C_train, A_unknown, nLatentVariables) returns
    %   concentration matrix C_pls computed using the weights and loadings
    %   from the SIMPLS algorithm on mean-centered A_train and C_train.
    %   The relationship between multiplier matrix B_pls and C_pls is
    %   C_pls = (A_unknown - mean(A_train,1)) * B_pls + mean(C_train,1).
    %
    %   pnnl_pls(A_train, C_train, A_unknown, nLatentVariables, meanCentered) applies mean
    %   centering when meanCentered is true, and does not apply mean
    %   centering when meanCentered is false.  When meanCentered is not
    %   supplied, the default is false (no mean centering).
    %
    %   Example:
    %
    %     load pnnl_napalm_data
    %     nLatentVariables = 3;
    %     meanCentered = true;
    %     [C_pls, B_pls] = pnnl_pls(A_train, C_train, ...
    %                               A_unknown, nLatentVariables, meanCentered);
    %
    %   See also pnnl_cls, pnnl_pcr.

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    if nargin < 5
        meanCentered = false;
    end

    X = A_train;
    Y = C_train;
    if meanCentered
        X0 = X - mean(X,1);
        Y0 = Y - mean(Y,1);
    else
        X0 = X;
        Y0 = Y;
    end
```

```
        [X_loadings,Y_loadings,X_scores,Y_scores,Weights] = pnnl_simpls(X0,Y0,nLatentVariables); %#ok<AS

        B_pls = Weights * Y_loadings';

        if meanCentered
            C_pls = (A_unknown - mean(A_train,1)) * B_pls + mean(C_train,1);
        else
            C_pls = A_unknown * B_pls;
        end
    end
```

Concentration Data

The concentrations of the training data are in matrix `C_train` and the concentrations of the validation data are in matrix `C_validation`. Column 1 corresponds to the concentrations in constituent 1 (benzene). Column 2 corresponds to the concentrations in constituent 2 (polystyrene). Column 3 corresponds to the concentrations in constituent 3 (gasoline).

$$C_{\text{train}} = \begin{array}{cc} \begin{array}{rrr} \textit{benzene} & \textit{polystyrene} & \textit{gasoline} \end{array} & \\ \left[\begin{array}{rrr} 0 & 0 & 100.0000 \\ 5.1309 & 0 & 94.8691 \\ 10.0660 & 0 & 89.9300 \\ 20.1799 & 0 & 79.8201 \\ 40.0120 & 0 & 59.9878 \\ 59.9972 & 0 & 40.0028 \\ 79.8412 & 0 & 20.1588 \\ 89.8273 & 0 & 10.1727 \\ 100.0000 & 0 & 0 \\ 90.0264 & 9.9736 & 0 \\ 80.1375 & 19.8625 & 0 \\ 64.9950 & 35.0005 & 0 \\ 21.0228 & 45.9197 & 33.0575 \\ 49.9507 & 5.0599 & 44.9895 \\ 40.0182 & 20.0385 & 39.9433 \\ 40.0154 & 10.0036 & 49.9810 \\ 30.0059 & 10.0282 & 59.9659 \\ 40.0340 & 39.9670 & 19.9990 \\ 49.9393 & 3.3748 & 46.6859 \\ 46.6501 & 13.4658 & 39.8840 \end{array}\right] & \begin{array}{r} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \end{array} \end{array}$$

$$C_{\text{validation}} = \begin{array}{cc} \begin{array}{rrr} \textit{benzene} & \textit{polystyrene} & \textit{gasoline} \end{array} & \\ \left[\begin{array}{rrr} 22.1665 & 39.0384 & 38.7951 \\ 21.6874 & 37.0596 & 41.2530 \\ 22.1665 & 39.6980 & 38.1355 \\ 26.9575 & 40.3576 & 32.6849 \\ 25.9993 & 33.7616 & 40.2391 \\ 23.1247 & 37.0596 & 39.8157 \\ 22.6456 & 39.0384 & 38.3160 \\ 22.6456 & 39.0384 & 38.3160 \\ 27.4366 & 42.3364 & 30.2270 \\ 27.4366 & 37.7192 & 34.8442 \\ 26.4784 & 40.3576 & 33.1640 \\ 26.9575 & 37.7192 & 35.3233 \end{array}\right] & \begin{array}{r} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \end{array} \end{array}$$

Clear variables and load the PNNL napalm data.

```
clearvars
load pnnl_napalm_data
```

PLS-2 with and without pre-processing

Choose the number of latent variables.

```
nLatentVariables = 3;
```

Set meanCentered to true to indicate that pre-processing (mean centering) is done, and false to indicate that pre-processing (mean centering) is not done.

```
for meanCentered = [true, false]
```

Set up the plot title and color.

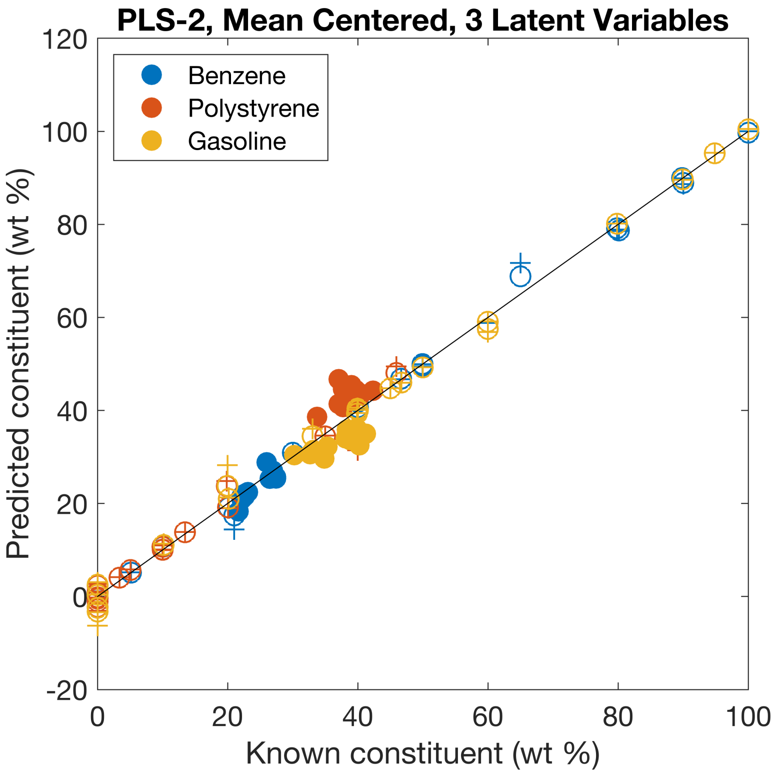
```
    LogicalStr = {'Not ',''};
    title_string = sprintf('PLS-2, %sMean Centered, %d Latent Variables',LogicalStr{mea
    nConstituents = size(C_validation,2);
    colorOrder = pnnl_colorOrder(nConstituents);
```

Use all the columns of C_train to compute PLS-2. Use all the columns of C_validation to compute RMSEP (root mean square error predicted). Use the columns of C_train to compute RMSEC (root mean square error calibration) and RMSECV (root mean square error cross validation).

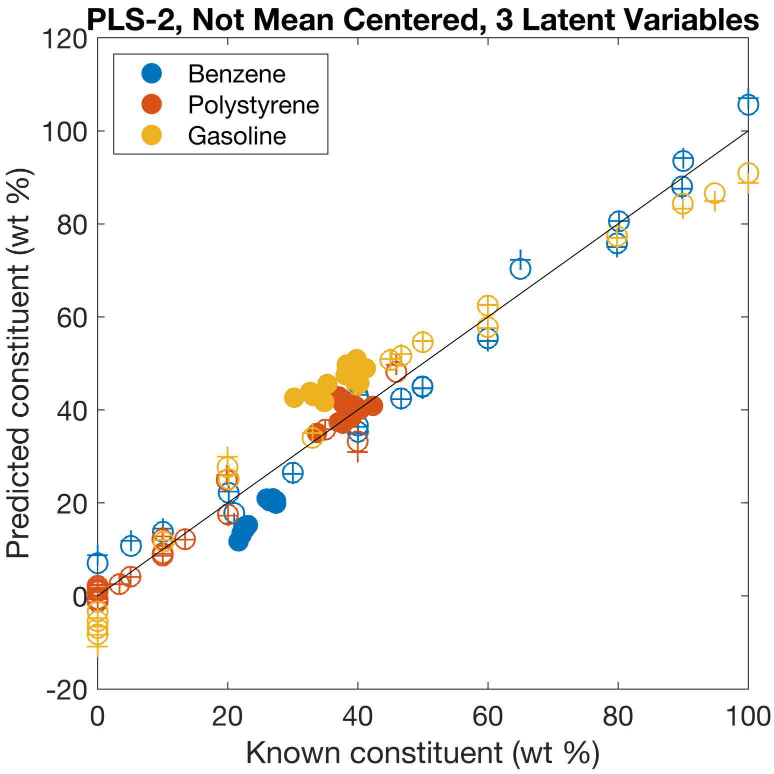
```
    % Compute PLS-2
    C_predicted = pnnl_pls(A_train,C_train,A_unknown,nLatentVariables,meanCentered);
    C_calibration = pnnl_pls(A_train,C_train,A_train,nLatentVariables,meanCentered);
    C_cross_validation = pnnl_cross_validation(@pnnl_pls,A_train,C_train,nLatentVariab
    % Compute RMSE
    RMSEP = pnnl_rmse(C_validation,C_predicted);
    RMSEC = pnnl_rmse(C_train,C_calibration);
    RMSECV = pnnl_rmse(C_train,C_cross_validation);
    % Display RMSE
    pnnl_display_rmse(title_string,ConstituentNames,RMSEC,RMSECV,RMSEP);

    % Plot results
    figure
    h = gobjects(nConstituents,1);
    for k = 1:nConstituents
        % Plot Concentrations
        hold on
        % Validation vs. Predicted
        h(k) = plot(C_validation(:,k),C_predicted(:,k),'.','MarkerSize',35,'Color',col
        % Train vs. Calibration
        plot(C_train(:,k),C_calibration(:,k),'o','MarkerSize',10,'LineWidth',1,'Color'
        % Train vs. Crosss Validation
        plot(C_train(:,k),C_cross_validation(:,k),'+','MarkerSize',10,'LineWidth',1,'C
        % 1-1 line
        line(C_train(:,k),C_train(:,k),'Color','k')
        title(title_string)
        xlabel(['Known constituent (',ConcentrationUnits,')'])
        ylabel(['Predicted constituent (',ConcentrationUnits,')'])
        set(gca,'FontSize',14)
        box on
        axis square
        hold off
    end
    legend(h,'Location','northwest')
    disp('Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.'
end
```

```
--------------------------------------------------------------------------------------
  PLS-2, Mean Centered, 3 Latent Variables       Benzene   Polystyrene      Gasoline
                                     RMSEC        1.3968        1.8465        1.5789
                                    RMSECV        2.2406        2.6176        2.7657
                                     RMSEP        1.6799        5.0647        4.2528
--------------------------------------------------------------------------------------
```



```
Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.
------------------------------------------------------------------------------------------
  PLS-2, Not Mean Centered, 3 Latent Variables       Benzene   Polystyrene      Gasoline
                                         RMSEC        4.1853        2.3592        5.6109
                                        RMSECV        5.0232        2.9897        6.6976
                                         RMSEP        7.5851        2.2404        9.8369
------------------------------------------------------------------------------------------
```



Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.

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